

## SESSION A'2: SYMPOSIUM OF THE DIVISION OF CONDENSED MATTER PHYSICS: EPITAXY INDUCED STRUCTURES

Monday morning, 20 March 1989; Room 132 at 9:12; A. Zangwill, presiding

9:12

**A'2 1 Stabilization of Epitaxial Structures. DAVID M. WOOD, SERI.**

Phenomena peculiar to coherent epitaxial growth of alloys include: (i) ordered compounds not present in the bulk phase diagram; (ii) constituents insoluble in bulk below a miscibility temperature  $T_G$  become epitaxially soluble even 1200 °C lower; (iii) the pinning of the measured composition  $x$  of an **epitaxial** alloy near where the alloy is lattice matched to the substrate ('lattice latching' or 'pulling'), while the composition  $x$  of a **bulk** alloy grown under identical conditions varies widely. A simple picture of epitaxial energetics makes clear the origin of these effects. A cluster-based theoretical description permits prediction and quantitative comparison of bulk and epitaxial  $(x,T)$  phase diagrams for the same system. It also places the common phenomenological treatment of an alloy as an elastic continuum on a microscopic footing (and highlights its inadequacies!). Results will be given for (a)  $\text{Cu}_{1-x}\text{Au}_x$ , a typical 'ordering' alloy (with stable stoichiometric compounds in bulk) and (b) the isovalent semiconductor  $\text{GaAs}_x\text{Sb}_{1-x}$ , a typical 'Phase separating' alloy (insoluble until entropy dominates above  $T_{MC}$ ). All of the effects above emerge naturally from our treatment; we trace them to the lattice mismatch between the alloy constituents, not to mismatch with the substrate. A simple expression relates the degree of composition pinning to the epitaxial suppression of the miscibility temperature. Using an epitaxial generalization of a recent thermodynamic treatment of bulk molecular beam epitaxy growth of  $\text{A}_{1-x}\text{B}_x\text{C}$  isovalent semiconductors<sup>3</sup> we demonstrate that composition pinning should be observable here as well. Substrate orientation and film thickness effects will also be discussed.

<sup>1</sup>D. M. Wood and Alex Zunger, Phys. Rev. Lett. 61, 1501 (1988).

<sup>2</sup>D. M. Wood and Alex Zunger, Phys. Rev. **B38** (in press).

<sup>3</sup>I. Seki and A. Koukitu, J. Cryst. Growth 78, 342 (1986).